



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:28 PM UTC

PDB ID : 3A70 / pdb_00003a70
Title : Crystal structure of Pseudomonas sp. MIS38 lipase in complex with diethyl phosphate
Authors : Angkawidjaja, C.; Matsumura, H.; Koga, Y.; Takano, K.; Kanaya, S.
Deposited on : 2009-09-10
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

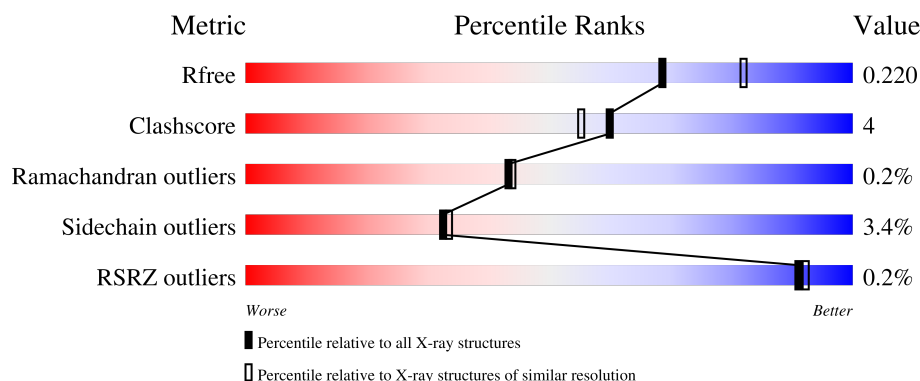
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	617	 86% 11% ..
1	C	617	 88% 11% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10224 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

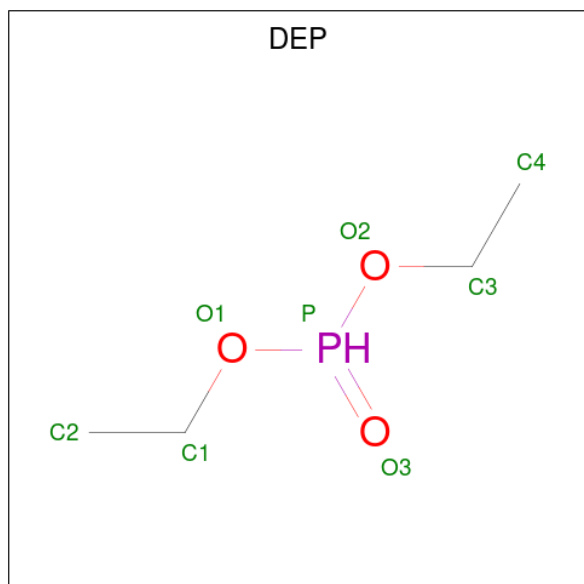
- Molecule 1 is a protein called Lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	0	0	0
			4484	2812	759	908	5			
1	C	616	Total	C	N	O	S	0	0	0
			4553	2863	769	916	5			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

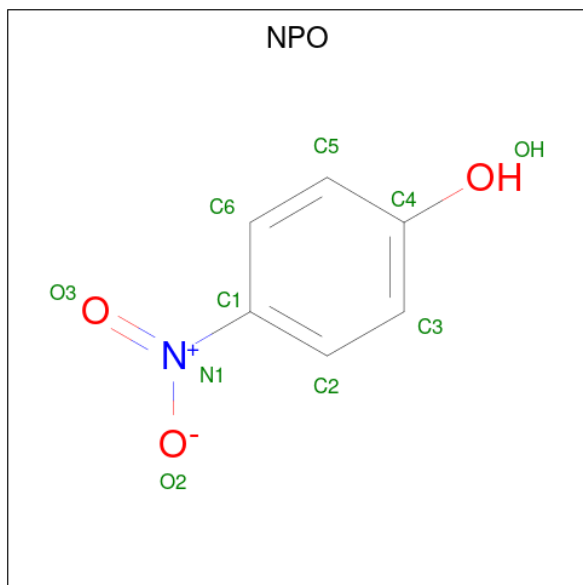
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	11	Total	Ca	0	0
			11	11		
2	C	11	Total	Ca	0	0
			11	11		

- Molecule 3 is DIETHYL PHOSPHONATE (CCD ID: DEP) (formula: C₄H₁₁O₃P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			8	4	3	1		
3	C	1	Total	C	O	P	0	0
			8	4	3	1		

- Molecule 4 is P-NITROPHENOL (CCD ID: NPO) (formula: $C_6H_5NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	6	1	3		
4	C	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

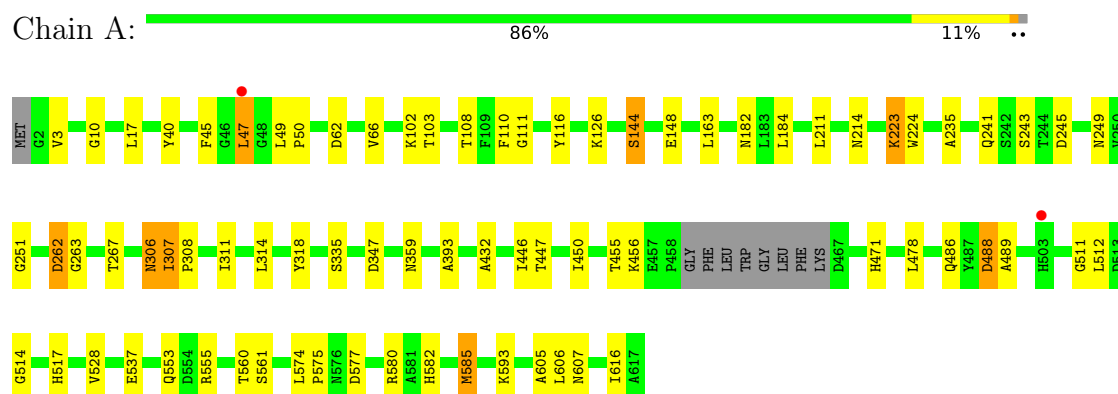
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	566	Total	O	0	0
			566	566		
6	C	555	Total	O	0	0
			555	555		

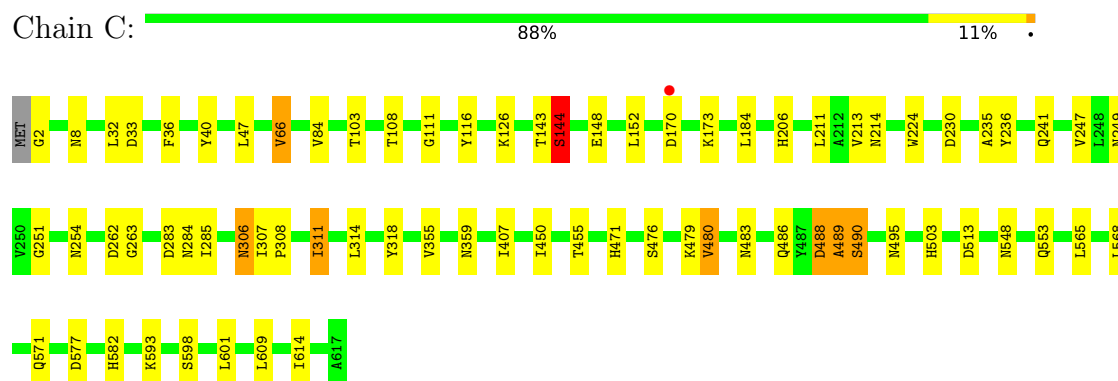
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Lipase



• Molecule 1: Lipase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	104.30Å 104.30Å 496.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.91 – 2.15 31.91 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (31.91-2.15) 99.2 (31.91-2.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.170 , 0.222 0.170 , 0.220	Depositor DCC
R_{free} test set	4393 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10224	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DEP, CA, ACT, NPO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.13	11/4574 (0.2%)	1.07	12/6214 (0.2%)
1	C	1.08	7/4648 (0.2%)	1.04	6/6315 (0.1%)
All	All	1.11	18/9222 (0.2%)	1.05	18/12529 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	512	LEU	C-O	-8.36	1.13	1.24
1	C	307	ILE	CA-CB	7.76	1.59	1.53
1	A	511	GLY	C-O	-6.67	1.16	1.23
1	A	307	ILE	CA-CB	6.65	1.58	1.53
1	A	514	GLY	C-O	-6.62	1.16	1.23
1	A	528	VAL	CA-CB	6.49	1.60	1.53
1	C	283	ASP	C-O	-6.45	1.15	1.24
1	A	446	ILE	CA-CB	6.24	1.61	1.54
1	A	144	SER	C-O	-6.12	1.16	1.24
1	C	247	VAL	CA-CB	5.95	1.61	1.54
1	C	489	ALA	CA-CB	5.86	1.62	1.53
1	A	488	ASP	CA-C	5.64	1.59	1.52
1	C	144	SER	C-O	-5.62	1.16	1.24
1	A	393	ALA	CA-CB	-5.40	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	432	ALA	CA-CB	5.36	1.60	1.53
1	C	355	VAL	CA-CB	5.29	1.60	1.53
1	A	267	THR	CA-CB	5.19	1.61	1.53
1	C	284	ASN	CG-OD1	-5.03	1.14	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	ASP	CA-C-N	10.65	131.96	120.03
1	A	262	ASP	C-N-CA	10.65	131.96	120.03
1	C	480	VAL	CB-CA-C	-9.68	100.35	111.09
1	A	488	ASP	CB-CA-C	6.09	119.83	109.72
1	A	148	GLU	CB-CA-C	-5.82	100.78	110.68
1	A	560	THR	CA-C-N	5.76	128.27	120.38
1	A	560	THR	C-N-CA	5.76	128.27	120.38
1	C	148	GLU	CB-CA-C	-5.63	99.53	110.46
1	C	247	VAL	N-CA-C	5.57	115.88	107.80
1	A	306	ASN	CA-C-N	5.51	123.71	120.24
1	A	306	ASN	C-N-CA	5.51	123.71	120.24
1	C	285	ILE	N-CA-C	5.43	115.91	107.99
1	A	514	GLY	N-CA-C	-5.37	105.83	112.33
1	C	571	GLN	N-CA-C	5.30	117.92	110.23
1	C	488	ASP	CB-CA-C	5.18	118.88	109.62
1	A	347	ASP	CA-C-N	-5.12	113.65	119.28
1	A	347	ASP	C-N-CA	-5.12	113.65	119.28
1	A	262	ASP	O-C-N	-5.01	116.50	123.12

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	262	ASP	Peptide
1	C	262	ASP	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4484	0	4268	35	0
1	C	4553	0	4338	41	0
2	A	11	0	0	0	0
2	C	11	0	0	0	0
3	A	8	0	10	1	0
3	C	8	0	10	0	0
4	A	10	0	5	1	0
4	C	10	0	4	2	0
5	A	4	0	3	0	0
5	C	4	0	3	0	0
6	A	566	0	0	11	0
6	C	555	0	0	11	0
All	All	10224	0	8641	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (77) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ASP:HB2	6:C:1181:HOH:O	1.57	1.05
1:A:10:GLY:HA3	6:A:1145:HOH:O	1.63	0.99
1:C:306:ASN:ND2	1:C:308:PRO:HD2	1.81	0.95
1:C:306:ASN:HD22	1:C:308:PRO:HD2	1.41	0.84
1:A:214:ASN:HD21	1:A:249:ASN:HD21	1.26	0.80
1:A:40:TYR:CE1	1:A:311:ILE:HD11	2.16	0.80
1:C:33:ASP:HA	4:C:630:NPO:H3	1.64	0.79
1:C:214:ASN:HD21	1:C:249:ASN:HD21	1.30	0.77
1:C:483:ASN:HB3	6:C:1152:HOH:O	1.86	0.74
1:A:241:GLN:OE1	1:A:263:GLY:HA2	1.90	0.71
1:C:577:ASP:OD2	1:C:582:HIS:HE1	1.73	0.71
3:A:629:DEP:H21	4:A:630:NPO:O3	1.91	0.70
1:A:306:ASN:ND2	1:A:308:PRO:HD2	2.05	0.70
1:C:170:ASP:HA	6:C:1447:HOH:O	1.91	0.70
1:A:306:ASN:HD22	1:A:308:PRO:HD2	1.57	0.69
1:A:47:LEU:O	1:A:50:PRO:HD2	1.93	0.69
1:C:471:HIS:HD2	6:C:1157:HOH:O	1.76	0.67
1:C:33:ASP:HB3	4:C:630:NPO:H2	1.75	0.67
1:C:40:TYR:CE1	1:C:311:ILE:HD11	2.35	0.62
1:A:10:GLY:CA	6:A:1145:HOH:O	2.34	0.60
1:C:36:PHE:CD2	1:C:314:LEU:HD11	2.36	0.60
1:A:555:ARG:NH2	6:A:953:HOH:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:LYS:HD3	6:C:1273:HOH:O	2.01	0.59
1:C:241:GLN:OE1	1:C:263:GLY:HA2	2.02	0.59
1:C:503:HIS:HB2	6:C:1131:HOH:O	2.02	0.59
1:A:182:ASN:HB3	6:A:1199:HOH:O	2.02	0.58
1:A:251:GLY:HA2	1:A:318:TYR:HE1	1.69	0.57
1:C:577:ASP:OD2	1:C:582:HIS:CE1	2.57	0.55
1:C:455:THR:OG1	1:C:471:HIS:HE1	1.92	0.53
1:A:245:ASP:HB3	6:A:1290:HOH:O	2.08	0.52
1:C:170:ASP:HB3	6:C:1449:HOH:O	2.08	0.52
1:C:306:ASN:HD22	1:C:306:ASN:C	2.18	0.52
1:C:495:ASN:HD22	1:C:513:ASP:H	1.58	0.52
1:A:455:THR:OG1	1:A:471:HIS:HE1	1.93	0.51
1:C:582:HIS:HD2	1:C:593:LYS:O	1.95	0.50
1:C:170:ASP:HB2	1:C:173:LYS:HB3	1.95	0.49
1:A:223:LYS:NZ	6:A:1332:HOH:O	2.43	0.49
1:A:184:LEU:HD12	1:A:224:TRP:CZ2	2.49	0.48
1:C:143:THR:O	1:C:144:SER:CB	2.62	0.48
1:A:585:MET:HE2	1:A:606:LEU:H	1.78	0.48
1:A:580:ARG:HD2	6:A:1238:HOH:O	2.14	0.47
1:C:235:ALA:HB3	1:C:249:ASN:ND2	2.28	0.47
1:C:565:LEU:HD11	1:C:601:LEU:HD21	1.96	0.47
1:A:574:LEU:O	1:A:575:PRO:C	2.56	0.47
1:C:553:GLN:NE2	1:C:598:SER:OG	2.47	0.47
1:A:211:LEU:C	1:A:211:LEU:HD23	2.41	0.46
1:A:471:HIS:HB3	1:A:478:LEU:HB3	1.98	0.46
1:C:489:ALA:HB3	6:C:1451:HOH:O	2.16	0.46
1:C:2:GLY:N	6:C:725:HOH:O	2.48	0.46
1:A:103:THR:HA	1:A:108:THR:O	2.16	0.46
1:A:111:GLY:HA3	1:A:116:TYR:O	2.16	0.46
1:A:585:MET:HE2	6:A:1146:HOH:O	2.14	0.45
1:C:36:PHE:CD2	1:C:36:PHE:C	2.94	0.45
1:A:582:HIS:HD2	1:A:593:LYS:O	1.99	0.45
1:C:111:GLY:HA3	1:C:116:TYR:O	2.16	0.45
1:A:45:PHE:CD1	1:A:49:LEU:HD13	2.52	0.45
1:A:447:THR:HB	1:A:450:ILE:HD12	1.98	0.44
1:C:103:THR:HA	1:C:108:THR:O	2.16	0.44
1:C:251:GLY:HA2	1:C:318:TYR:HE1	1.81	0.44
1:A:102:LYS:HD2	1:A:110:PHE:CG	2.53	0.44
1:C:609:LEU:HD22	1:C:614:ILE:HD11	1.99	0.44
1:A:489:ALA:HB3	6:A:1130:HOH:O	2.17	0.44
1:C:407:ILE:HG22	1:C:450:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:ASP:OD2	1:A:582:HIS:HE1	2.00	0.44
1:A:561:SER:HB2	6:A:717:HOH:O	2.18	0.43
1:A:62:ASP:OD1	6:A:833:HOH:O	2.22	0.43
1:A:585:MET:HE1	1:A:605:ALA:HA	2.01	0.43
1:C:254:ASN:HB3	6:C:783:HOH:O	2.19	0.43
1:A:517:HIS:NE2	1:A:537:GLU:OE2	2.40	0.42
1:C:32:LEU:HD11	1:C:66:VAL:HG22	2.02	0.42
1:C:206:HIS:HA	1:C:236:TYR:O	2.19	0.42
1:C:548:ASN:HA	1:C:568:LEU:O	2.20	0.41
1:C:490:SER:HB2	6:C:711:HOH:O	2.20	0.41
1:A:235:ALA:HB3	1:A:249:ASN:ND2	2.35	0.41
1:C:213:VAL:HB	1:C:235:ALA:HB2	2.03	0.41
1:C:184:LEU:HD12	1:C:224:TRP:CZ2	2.56	0.41
1:A:3:VAL:HA	1:A:335:SER:C	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	604/617 (98%)	592 (98%)	11 (2%)	1 (0%)	43	44
1	C	614/617 (100%)	597 (97%)	16 (3%)	1 (0%)	43	44
All	All	1218/1234 (99%)	1189 (98%)	27 (2%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	144	SER
1	A	144	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	464/471 (98%)	447 (96%)	17 (4%)	30	30
1	C	470/471 (100%)	455 (97%)	15 (3%)	34	36
All	All	934/942 (99%)	902 (97%)	32 (3%)	32	33

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	47	LEU
1	A	66	VAL
1	A	126	LYS
1	A	163	LEU
1	A	223	LYS
1	A	243	SER
1	A	307	ILE
1	A	314	LEU
1	A	359	ASN
1	A	456	LYS
1	A	486	GLN
1	A	488	ASP
1	A	553	GLN
1	A	585	MET
1	A	607	ASN
1	A	616	ILE
1	C	8	ASN
1	C	47	LEU
1	C	66	VAL
1	C	84	VAL
1	C	126	LYS
1	C	152	LEU
1	C	211	LEU
1	C	306	ASN
1	C	311	ILE
1	C	359	ASN

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Mol	Chain	Res	Type
1	C	476	SER
1	C	480	VAL
1	C	486	GLN
1	C	488	ASP
1	C	490	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	43	ASN
1	A	130	GLN
1	A	160	ASN
1	A	249	ASN
1	A	306	ASN
1	A	471	HIS
1	A	495	ASN
1	A	553	GLN
1	A	582	HIS
1	C	8	ASN
1	C	96	GLN
1	C	160	ASN
1	C	249	ASN
1	C	306	ASN
1	C	471	HIS
1	C	495	ASN
1	C	553	GLN
1	C	582	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 22 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NPO	C	630	-	10,10,10	2.38	6 (60%)	11,13,13	1.32	1 (9%)
4	NPO	A	630	-	10,10,10	0.89	0	11,13,13	0.65	0
5	ACT	A	631	-	3,3,3	0.79	0	3,3,3	1.55	0
3	DEP	A	629	1	4,7,7	0.63	0	2,7,7	0.67	0
5	ACT	C	631	-	3,3,3	0.81	0	3,3,3	1.48	0
3	DEP	C	629	1	4,7,7	0.60	0	2,7,7	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NPO	A	630	-	-	0/2/4/4	0/1/1/1
3	DEP	A	629	1	-	0/2/6/6	-
4	NPO	C	630	-	-	1/2/4/4	0/1/1/1
3	DEP	C	629	1	-	0/2/6/6	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	630	NPO	C1-N1	-3.89	1.36	1.45
4	C	630	NPO	C2-C1	-2.86	1.33	1.38
4	C	630	NPO	O3-N1	-2.66	1.18	1.22
4	C	630	NPO	C3-C4	-2.50	1.34	1.39
4	C	630	NPO	O2-N1	-2.37	1.19	1.35
4	C	630	NPO	OH-C4	-2.15	1.32	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	C	630	NPO	O3-N1-C1	-2.85	114.90	118.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	630	NPO	C2-C1-N1-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	630	NPO	2	0
4	A	630	NPO	1	0
3	A	629	DEP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	608/617 (98%)	-0.57	2 (0%) 90 91	11, 18, 32, 53	0
1	C	616/617 (99%)	-0.43	1 (0%) 91 92	11, 20, 35, 52	0
All	All	1224/1234 (99%)	-0.50	3 (0%) 91 92	11, 19, 33, 53	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	LEU	2.5
1	A	503	HIS	2.2
1	C	170	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	A	631	4/4	0.60	0.25	73,73,73,73	0
5	ACT	C	631	4/4	0.75	0.26	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NPO	C	630	10/10	0.80	0.25	75,75,76,77	0
4	NPO	A	630	10/10	0.83	0.23	62,65,67,67	0
3	DEP	C	629	8/8	0.98	0.06	17,23,23,23	0
2	CA	A	620	1/1	0.98	0.02	14,14,14,14	0
2	CA	C	625	1/1	0.98	0.03	31,31,31,31	0
2	CA	C	626	1/1	0.98	0.04	24,24,24,24	0
3	DEP	A	629	8/8	0.98	0.06	9,17,19,24	0
2	CA	C	623	1/1	0.99	0.03	24,24,24,24	0
2	CA	C	624	1/1	0.99	0.02	23,23,23,23	0
2	CA	A	618	1/1	0.99	0.02	14,14,14,14	0
2	CA	A	622	1/1	0.99	0.09	22,22,22,22	0
2	CA	C	627	1/1	0.99	0.03	35,35,35,35	0
2	CA	C	628	1/1	0.99	0.02	19,19,19,19	0
2	CA	A	623	1/1	0.99	0.01	18,18,18,18	0
2	CA	A	626	1/1	0.99	0.02	15,15,15,15	0
2	CA	A	627	1/1	0.99	0.04	28,28,28,28	0
2	CA	C	619	1/1	0.99	0.03	20,20,20,20	0
2	CA	C	621	1/1	0.99	0.01	16,16,16,16	0
2	CA	C	622	1/1	0.99	0.06	21,21,21,21	0
2	CA	A	625	1/1	1.00	0.01	20,20,20,20	0
2	CA	A	619	1/1	1.00	0.02	17,17,17,17	0
2	CA	A	621	1/1	1.00	0.02	14,14,14,14	0
2	CA	A	628	1/1	1.00	0.03	15,15,15,15	0
2	CA	C	618	1/1	1.00	0.01	16,16,16,16	0
2	CA	A	624	1/1	1.00	0.02	13,13,13,13	0
2	CA	C	620	1/1	1.00	0.01	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.